

On a special property of tridiagonal matrices. Application to dual quasi-exactly solvable sextic potentials in quantum mechanics

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Abstract

We put forward and prove a simple theorem stating that the eigenvalues of a tridiagonal matrix change their sign (as a set), once the signs of the diagonal elements of the matrix are changed. We also provide an example of application of this theorem in quantum physics. Specifically, we introduce the notion of duality and self-duality for a sextic-polynomial quasi-exactly-solvable potential, and demonstrate that the algebraic parts of the spectrum of the dual potentials have signs opposite to one another (as sets). Our Theorem furnishes an elegant one-line proof of this statement. In addition, we also prove it by purely quantum-mechanical means — a far less straightforward method that requires some effort.

Introduction

Tridiagonal matrices naturally emerge in various fields of mathematics, physics and other sciences. We shall prove a theorem relating the spectra of tridiagonal matrices with opposite elements on their diagonals. Motivation for this study comes from quantum mechanics. Stationary problems of quantum mechanics, typically, fall into one of the two large categories: the problems are either exactly solvable (so the spectrum and the wave functions can be found analytically) or are unsolvable by analytical means. However, in the late 1980-s an intermediate class of problems was discovered — the quasi-exactly solvable (QES) problems [1–4]. These settings permit analytic derivation of a finite part of the (generally, infinite) spectrum, by partial reducing of the Hamiltonian to a block-diagonal form.

In [5], two dual QES periodic potentials were considered, whose spectra interchange under the switch $E \rightarrow -E$, where E is the energy. In the self-dual case, when the two potentials are equal to each other, the spectrum transforms into itself under the said switch.

In [6,7], it was noticed that *the algebraic (i.e., analytically derivable) part* of the spectrum of a sextic QES potential transforms into itself under the switch $E \rightarrow -E$. In this, restricted sense, such a potential can be regarded self-dual. Accordingly, it is natural to hypothesise that there also exist dual sextic potentials whose algebraic parts of spectra interchange under $E \rightarrow -E$. Here we discuss such potentials and demonstrate the symmetry of their spectra, using a Theorem proven in Section 1.

In addition to this, we present an independent, quantum-mechanical proof of the mentioned symmetry of the spectra.

1 The eigenvalues of a general-form tridiagonal matrix

Lemma. *Let M and \widetilde{M} be tridiagonal matrices:*

$$M_n = \begin{pmatrix} a_1 & b_1 & 0 & 0 \\ c_1 & a_2 & \ddots & 0 \\ 0 & \ddots & \ddots & b_{n-1} \\ 0 & 0 & c_{n-1} & a_n \end{pmatrix}, \quad \widetilde{M}_n = \begin{pmatrix} -a_1 & b_1 & 0 & 0 \\ c_1 & -a_2 & \ddots & 0 \\ 0 & \ddots & \ddots & b_{n-1} \\ 0 & 0 & c_{n-1} & -a_n \end{pmatrix}. \quad (1)$$

Then their determinants, in the case of an odd and even n , are related, correspondingly, as:

$$\det \widetilde{M}_{2k-1} = -\det M_{2k-1}, \quad \det \widetilde{M}_{2k} = \det M_{2k}. \quad (2)$$

Proof. (By induction) For $k = 1$, the two above formulae are straightforward:

$$\det(-a_1) = -\det(a_1), \quad \det \begin{pmatrix} -a_1 & b_1 \\ c_1 & -a_2 \end{pmatrix} = (-a_1)(-a_2) - b_1 c_1 = a_1 a_2 - b_1 c_1 = \det \begin{pmatrix} a_1 & b_1 \\ c_1 & a_2 \end{pmatrix}. \quad (3)$$

Now assume the fulfilment of the formulae (2) for $k = m - 1$. Then, for $k = m$, one has:

$$\begin{aligned}
\det \widetilde{M}_{2m-1} &= \begin{vmatrix} -a_1 & b_1 & 0 & 0 \\ c_1 & -a_2 & \ddots & 0 \\ 0 & \ddots & \ddots & b_{2m-2} \\ 0 & 0 & c_{2m-2} & -a_{2m-1} \end{vmatrix}_{2m-1} = -a_1 \begin{vmatrix} -a_2 & b_2 & 0 & 0 \\ c_2 & -a_3 & \ddots & 0 \\ 0 & \ddots & \ddots & b_{2m-2} \\ 0 & 0 & c_{2m-2} & -a_{2m-1} \end{vmatrix}_{2m-2} \\
&\quad -b_1 \begin{vmatrix} c_1 & b_2 & 0 & 0 \\ 0 & -a_3 & \ddots & 0 \\ 0 & \ddots & \ddots & b_{2m-2} \\ 0 & 0 & c_{2m-2} & -a_{2m-1} \end{vmatrix}_{2m-2} = -a_1 \begin{vmatrix} -a_2 & b_2 & 0 & 0 \\ c_2 & -a_3 & \ddots & 0 \\ 0 & \ddots & \ddots & b_{2m-2} \\ 0 & 0 & c_{2m-1} & -a_{2m-1} \end{vmatrix}_{2m-2} \\
&\quad -b_1 \left(\begin{vmatrix} -a_3 & b_3 & 0 & 0 \\ c_3 & -a_4 & \ddots & 0 \\ 0 & \ddots & \ddots & b_{2m-2} \\ 0 & 0 & c_{2m-2} & -a_{2m-1} \end{vmatrix}_{2m-3} -b_2 \begin{vmatrix} 0 & b_3 & 0 & 0 \\ 0 & -a_4 & \ddots & 0 \\ 0 & \ddots & \ddots & b_{2m-2} \\ 0 & 0 & c_{2m-2} & -a_{2m-1} \end{vmatrix}_{2m-3} \right) \\
&\stackrel{\text{By assumption}}{=} - \left(a_1 \begin{vmatrix} a_2 & b_2 & 0 & 0 \\ c_2 & a_3 & \ddots & 0 \\ 0 & \ddots & \ddots & b_{2m-2} \\ 0 & 0 & c_{2m-2} & a_{2m-1} \end{vmatrix}_{2m-2} -b_1 c_1 \begin{vmatrix} a_3 & b_3 & 0 & 0 \\ c_3 & a_4 & \ddots & 0 \\ 0 & \ddots & \ddots & b_{2m-2} \\ 0 & 0 & c_{2m-2} & a_{2m-1} \end{vmatrix}_{2m-3} \right) = -\det M_{2m-1}
\end{aligned} \tag{4}$$

and, similarly:

$$\begin{aligned}
\det \widetilde{M}_{2m} &= \begin{vmatrix} -a_1 & b_1 & 0 & 0 \\ c_1 & -a_2 & \ddots & 0 \\ 0 & \ddots & \ddots & b_{2m-1} \\ 0 & 0 & c_{2m-1} & -a_{2m} \end{vmatrix}_{2m} = -a_1 \begin{vmatrix} -a_2 & b_2 & 0 & 0 \\ c_2 & -a_3 & \ddots & 0 \\ 0 & \ddots & \ddots & b_{2m} \\ 0 & 0 & c_{2m} & -a_{2m} \end{vmatrix}_{2m-1} \\
&\quad -b_1 \begin{vmatrix} c_1 & b_2 & 0 & 0 \\ 0 & -a_3 & \ddots & 0 \\ 0 & \ddots & \ddots & b_{2m-1} \\ 0 & 0 & c_{2m-1} & -a_{2m} \end{vmatrix}_{2m-1} = -a_1 \begin{vmatrix} -a_2 & b_2 & 0 & 0 \\ c_2 & -a_3 & \ddots & 0 \\ 0 & \ddots & \ddots & b_{2m-1} \\ 0 & 0 & c_{2m-1} & -a_{2m} \end{vmatrix}_{2m-1} \\
&\quad -b_1 \left(c_1 \begin{vmatrix} -a_3 & b_3 & 0 & 0 \\ c_3 & -a_4 & \ddots & 0 \\ 0 & \ddots & \ddots & b_{2m-1} \\ 0 & 0 & c_{2m-1} & -a_{2m} \end{vmatrix}_{2m-2} - b_2 \begin{vmatrix} 0 & b_3 & 0 & 0 \\ 0 & -a_4 & \ddots & 0 \\ 0 & \ddots & \ddots & b_{2m-1} \\ 0 & 0 & c_{2m-1} & -a_{2m} \end{vmatrix}_{2m-2} \right) \\
&\stackrel{\text{By assumption}}{=} a_1 \begin{vmatrix} a_2 & b_2 & 0 & 0 \\ c_2 & a_3 & \ddots & 0 \\ 0 & \ddots & \ddots & b_{2m-1} \\ 0 & 0 & c_{2m-1} & a_{2m} \end{vmatrix}_{2m-1} - b_1 c_1 \begin{vmatrix} a_3 & b_3 & 0 & 0 \\ c_3 & a_4 & \ddots & 0 \\ 0 & \ddots & \ddots & b_{2m-1} \\ 0 & 0 & c_{2m-1} & a_{2m} \end{vmatrix}_{2m-2} = \det M_{2m} \quad .
\end{aligned} \tag{5}$$

□

Aside from the rigorous proof, we can guess the above result via qualitative reasoning. The determinant of the matrix is, generally, a sum of $n!$ terms, each of which contains, at most, one multiplier a_k for each k . If the overall power of a_k 's in each term is odd (even), the determinant will (not) change the sign as we flip the signs of all a_k 's. This is exactly the case of tridiagonal matrices of an odd (even) size.

Theorem. Let $P_n(\lambda)$ and $\widetilde{P}_n(\lambda)$ be the characteristic polynomials of the tridiagonal matrices introduced in (1):

$$P_n(\lambda) = \det |M_n - \lambda \mathbf{1}| \quad , \quad \widetilde{P}_n(\lambda) = \det |\widetilde{M}_n - \lambda \mathbf{1}| \quad . \tag{6}$$

Then:

$$\widetilde{P}_{2k+1}(\lambda) = -P_{2k+1}(-\lambda) \quad , \quad \widetilde{P}_{2k}(\lambda) = P_{2k}(-\lambda) \quad . \tag{7}$$

Proof. The proof ensues immediately from the previous lemma, if one substitutes:

$$\begin{aligned}
a_m &\rightarrow -a_m - \lambda && \text{in } M_n \quad , \\
-a_m &\rightarrow -a_m - \lambda && \text{in } \widetilde{M}_n \quad .
\end{aligned} \tag{8}$$

□

One can formulate our result in a slightly different way:

Theorem. *If two tridiagonal matrices differ only by signs of their diagonal elements, then the sets of their eigenvalues can be obtained from one another by sign inversion.*

Proof. Indeed, the previous theorem states that the eigenvalues of M_n and \widetilde{M}_n can be found from the characteristic equations

$$\begin{aligned} M_n : \quad & P_n(\lambda) = 0 \quad , \\ \widetilde{M}_n : \quad & P_n(-\lambda) = 0 \quad . \end{aligned} \tag{9}$$

□

The following circumstance is worth noting. Suppose one has managed to derive the closed-form expressions for the roots of the $P_n(\lambda)$:

$$\lambda_k = f_k(a_1, \dots, a_n; b_1, \dots, b_{n-1}, c_1, \dots, c_{n-1}) \quad , \quad k = 1 \dots n \quad . \tag{10}$$

Generally, the individual roots will not simply change their signs under the change of the signs of a_k :

$$\widetilde{\lambda}_k = f_k(-a_1, \dots, -a_n; b_1, \dots, b_{n-1}, c_1, \dots, c_{n-1}) \neq -\lambda_k \quad , \quad k = 1 \dots n \quad . \tag{11}$$

However, the roots will change the sign as a set:

$$\{\lambda_1, \dots, \lambda_n\} \rightarrow \{\widetilde{\lambda}_1, \dots, \widetilde{\lambda}_n\} = \{-\lambda_1, \dots, -\lambda_n\} \quad . \tag{12}$$

2 An example from QM

2.1 Quasi-exact solvability, duality and self-duality

This section explains the motivation for the above result, and presents an instructive example of employment of the Theorem to some problems of Quantum Mechanics.

A wide range of classical systems with one degree of freedom can be described in the language of the Hamilton formalism. The equations of motion for such systems are:

$$\frac{dp}{dt} = -\frac{\partial H}{\partial q} \quad , \tag{13a}$$

$$\frac{dq}{dt} = \frac{\partial H}{\partial p} \quad , \tag{13b}$$

with the Hamiltonian taking the form of

$$H = \frac{p^2}{2m} + V(x) = E \quad . \tag{14}$$

As ever in the case of time-independent Hamiltonians, the value E of this Hamiltonian is conserved (and is termed the energy). From the latter equation, the canonical momentum can be written down as (below we shall use $m = 1$):

$$p(x, E) = \sqrt{2(E - V(x))} \quad . \tag{15}$$

The process of quantisation of a classical system can be thought of as replacing the classical position and momentum by operators obeying the canonical commutation relations:

$$[\hat{x}, \hat{p}] = i \hbar \quad , \quad (16)$$

and acting on the wave vectors ascribed to the states of a quantum system. Oftentimes, the so-called position representation is used:

$$x \rightarrow \hat{x} = x \quad , \quad p \rightarrow \hat{p} = -i \hbar \frac{d}{dx} \quad , \quad (17)$$

with the wave vectors implemented as functions of x . After the quantisation, the Hamiltonian becomes an operator, and the latter equality turns into a differential equation named after Erwin Schrödinger:

$$\hat{H} \psi(x) = \left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right] \psi(x) = E \psi(x) \quad . \quad (18)$$

To know the permissible energies, we need to find the spectrum of the differential operator \hat{H} . For bound states, the spectrum turns out to be discrete. These quantum states correspond to periodic motion in the classical system.¹ This is the only type of motion available for a potentials that become infinite at $|x| \rightarrow \infty$. For such motion, the process of solving the Schrödinger equation gets reduced to diagonalisation of a matrix of a countable but (generally) infinite size. There are few well-known *exactly solvable* problems, for which the entire matrix can be diagonalised. In general, this kind of problem cannot be solved analytically. However, there exist so-called *quasi-exactly solvable* (QES) problems, ones permitting partial algebraisation.² In these problems, the matrix of the Hamiltonian permits to single out a block of a finite size — which reduces the search of a limited number of energy levels to diagonalisation of a finite-sized matrix.

The most well-known examples of QES problems are the even and odd sixth-order polynomial potentials:³

$$V_{\text{even}}(\nu, \mu, j, x) = \frac{\nu^2}{8} x^6 + \frac{\mu \nu}{4} x^4 + \left[\frac{\mu^2}{8} - 2\nu \left(j + \frac{3}{8} \right) \right] x^2 - \mu \left(j + \frac{1}{4} \right) \quad , \quad (19a)$$

$$V_{\text{odd}}(\nu, \mu, j, x) = \frac{\nu^2}{8} x^6 + \frac{\mu \nu}{4} x^4 + \left[\frac{\mu^2}{8} - 2\nu \left(j + \frac{5}{8} \right) \right] x^2 - \mu \left(j + \frac{3}{4} \right) \quad , \quad (19b)$$

$$\nu \in \mathbb{R}^+, \quad , \quad \mu \in \mathbb{R} \quad , \quad j = 1/2, 1, 3/2, 2, \dots$$

These potentials are even and odd in the following sense. For them, the first $J = 2j+1$ lowest even (odd) energy levels can be obtained through diagonalisation of the following tridiagonal matrices:

¹ Bounded motion is necessarily periodic only in one-dimensional systems. For systems of higher dimensions, a more general statement is valid, the Poincaré recurrence theorem, see [8].

² For a detailed introduction into the topic, we would recommend [6] for a brief intro.

³ These potentials are discussed in [6]. Be mindful, though, that the constant parts of these potentials are omitted there.

$$\begin{aligned}
& \mathcal{H}_{\text{“G”}, \text{even}} : & \mathcal{H}_{\text{“G”}, \text{odd}} : \\
& \mathcal{H}_{k,k+1} = -k(2k-1) & \mathcal{H}_{k,k+1} = -k(2k+1) \\
& \mathcal{H}_{k,k} = \mu(k-j-1) & \mathcal{H}_{k,k} = \mu(k-j-1) \\
& \mathcal{H}_{k,k-1} = (k-2)\nu - 2j\nu & \mathcal{H}_{k,k-1} = (k-2)\nu - 2j\nu
\end{aligned} \quad k = 1, 2, \dots, J \quad . \quad (20)$$

This is owing to the fact that, after an eigenvalues-preserving quasi-gauge transformation,⁴ the Hamiltonians corresponding to potentials (19) can be written as:

$$H_{\text{“G”}, \text{even}} = -2T^0 T^- - (2j+1)T^- - \nu T^+ + \mu T^0 \quad , \quad (21a)$$

$$H_{\text{“G”}, \text{odd}} = -2T^0 T^- - (2j+1)T^- - \nu T^+ + \mu T^0 - 2T^- \quad , \quad (21b)$$

where the operators

$$\begin{aligned}
T^+ &= 2j\xi - \xi^2 \frac{d}{d\xi} \quad , & T^0 &= -j + \xi \frac{d}{d\xi} \quad , & T^- &= \frac{d}{d\xi} \quad , \\
& & \xi &= x^2
\end{aligned} \quad (22)$$

obey the commutation relation:

$$[T^+, T^-] = 2T^0 \quad , \quad [T^+, T^0] = -T^+ \quad , \quad [T^-, T^0] = T^- \quad (23)$$

and therefore can be interpreted as the generators of a representation of the $SU(2)$ group, with j being the spin and $J = 2j + 1$ the representation dimension. That the energies obtained through these means are the lowest ones of a given parity of the potential — that is warranted by the oscillation theorem [9] and by the fact that eigenfunctions of the operators (21) are polynomials in x^2 of powers from 0 to $2j$. (For an odd potential, an additional multiplier of x comes from the quasi-gauge transformation, see [6]).

For brevity, we introduce the notation

$$V_{\{\mu\}}(x) = V_{\text{even}}(\nu, \mu, j, x) \quad , \quad (24a)$$

$$\tilde{V}_{\{\mu\}}(x) = V_{\text{odd}}(\nu, \mu, j, x) \quad . \quad (24b)$$

The potentials with opposite values of the parameter μ possess the duality property:

$$V_{\{\mu\}}(x) = -V_{\{-\mu\}}(ix) \quad , \quad (25a)$$

$$\tilde{V}_{\{\mu\}}(x) = -\tilde{V}_{\{-\mu\}}(ix) \quad , \quad (25b)$$

⁴ Quasi-gauge is a transformation of the form $\psi(x) \rightarrow \psi_{\text{“G”}}(x) e^{-a(x)}$, $H \rightarrow e^{-a(x)} H_{\text{“G”}} e^{a(x)}$. The function $a(x)$ is set real, wherefore the transformation is *non-unitary*, and the norm of the wave function is not preserved. The physical meaning of such a transformation is straightforward: solutions to a one-dimensional Schrödinger equation are normally sought in the form of $(\sum_n a_n x^n) \exp(\dots)$ where the exponent defines the asymptotic behaviour. When the exponential is found somehow, it remains to determine the prefactor $\sum_n a_n x^n$. In special cases, this series truncates to a finite sum.

A key property of quasi-gauge transformations is that they preserve the eigenvalues of the operator. See [6] for details.

If one sets $\mu = 0$, this becomes the self-duality:

$$V_{\{0\}}(x) = -V_{\{0\}}(ix) \quad , \quad (26a)$$

$$\tilde{V}_{\{0\}}(x) = -\tilde{V}_{\{0\}}(ix) \quad . \quad (26b)$$

Effectively, it means that the motion in the potential $V_{\{-\mu\}}(x)$ can be considered as motion in $V_{\{\mu\}}(x)$ along the imaginary direction. For this reason, we will treat x as a complex variable.

In [6, 7], it was noticed that the algebraic parts of the spectra of potentials $V_{\{0\}}(x)$ and $\tilde{V}_{\{0\}}(x)$ are symmetric under the switch $E \rightarrow -E$. With the use of the Theorem proven in Section 1, it becomes straightforward from the equation (20) that this symmetry can be generalised to non-zero values of μ . In other words, the energies in the algebraic sector of the potentials (19) change their signs under $\mu \rightarrow -\mu$:

$$E_{\{\mu\},n} = -E_{\{-\mu\},N-n} \quad , \quad n = 0, 2, 4 \dots, N \quad (\text{for } V_{\text{even}}) \quad , \quad (27a)$$

$$\tilde{E}_{\{\mu\},\tilde{n}} = -\tilde{E}_{\{-\mu\},\tilde{N}+1-\tilde{n}} \quad , \quad \tilde{n} = 1, 3, 5 \dots, \tilde{N} \quad (\text{for } V_{\text{odd}}) \quad . \quad (27b)$$

Here N and \tilde{N} denote the highest energy levels in the algebraic sectors of the potentials:

$$N = 2J - 2 = 4j \quad , \quad (28a)$$

$$\tilde{N} = 2J - 1 = 4j + 1 \quad . \quad (28b)$$

2.2 The generalised Bohr-Sommerfeld quantisation condition

In this section, we provide an independent proof of the energy spectrum reflection symmetry (27). This proof will be purely quantum-mechanical, and will not rely on the algebraisation property (21) of the potentials. The section is largely based on the ideas proposed in [10].

To solve the Schrödinger equation (18), it is often convenient to change variables:

$$\psi(x) = \exp(i\sigma(x, E)/\hbar) \quad . \quad (29)$$

Then the function $\sigma(x)$ satisfies the Ricatti equation:

$$(\sigma'(x, E))^2 + \frac{\hbar}{i} \sigma''(x, E) = 2(E - V(x)) \quad . \quad (30)$$

In the limit $\hbar \rightarrow 0$, the function $\sigma'(x)$ becomes the classical momentum (15). So we shall name it the quantum momentum function (QMF), and shall introduce the notation

$$\varrho(x, E) = \sigma'(x, E) \quad (31)$$

in terms whereof the equation (30) will become

$$\varrho^2(x, E) + \frac{\hbar}{i} \varrho'(x, E) = 2(E - V(x)) \quad . \quad (32)$$

The quantisation condition determining the n -th energy level is normally obtained from the requirement of single-valuedness of the function $\psi(x)$. However, in [10] a more interesting option was proposed. It was based on the fact that the wave function corresponding to the n -th energy level has n zeros on the real axis, between the classical turning points (these points being the zeros of the classical momentum) [9].

In these zeroes, the QMF has poles. Indeed, it trivially follows from (29) and (31) that

$$\varrho(x, E) = \frac{\hbar}{i} \frac{1}{\psi(x)} \frac{d\psi(x)}{dx} \quad . \quad (33)$$

For analytic potentials, the pole of the function $\varrho(x)$ is of the first order, and the residue at this pole is $(-i\hbar)$. Therefore, the integral of the QMF along the contour \mathcal{C}_R enclosing classical turning points is:

$$\oint_{\mathcal{C}_R} \varrho(x, E) dx = 2\pi n \hbar \quad , \quad (34)$$

where the contour \mathcal{C}_R should be close enough to the real axis, in order to avoid containing the poles and branch cuts of $\varrho(x)$, that are off the real axis. Hereafter, we set $\hbar = 1$.

In the classical limit ($\hbar \rightarrow 0$), the series of poles inside \mathcal{C}_R coalesces into a branch cut of the classical momentum. The classical momentum is set positive along the bottom of the branch cut, in order for the classical action to stay positive when the direction of the contour in (34) is chosen to be counter-clockwise.

The subsequent discussion being applicable to both potentials presented in the equation (19), we shall concentrate on the even potential, equation (19a). Assume for the time being that the potential $V_{\{\mu\}}(x)$ is of a double-well shape (which is true for a wide range of the parameters), and that the equation

$$V_{\{\mu\}}(x) = E \quad (35)$$

has four solutions. In this case, the equation (34) reads as:

$$\oint_{\mathcal{C}_1} \varrho_{\{\mu\}}(x, E) dx = \oint_{\mathcal{C}_2} \varrho_{\{\mu\}}(x, E) dx = 2\pi m \quad . \quad (36)$$

where the contours are defined as in Figure 1.

From the equation (32), it follows that the duality property for the QMF has form:

$$\varrho_{\{-\mu\}}(x, -E) = i \varrho_{\{\mu\}}(ix, E) \quad . \quad (37)$$

It allows us to calculate the LHS of the (34) for the positive energy levels of the potential $V_{\{-\mu\}}(x)$ as an integral of $\varrho_{\{\mu\}}(x, E)$ along the imaginary axis:

$$\oint_{\mathcal{C}'_3} \varrho_{\{-\mu\}}(x, -E) dx = \oint_{\mathcal{C}_3} \varrho_{\{\mu\}}(x, E) dx \quad . \quad (38)$$

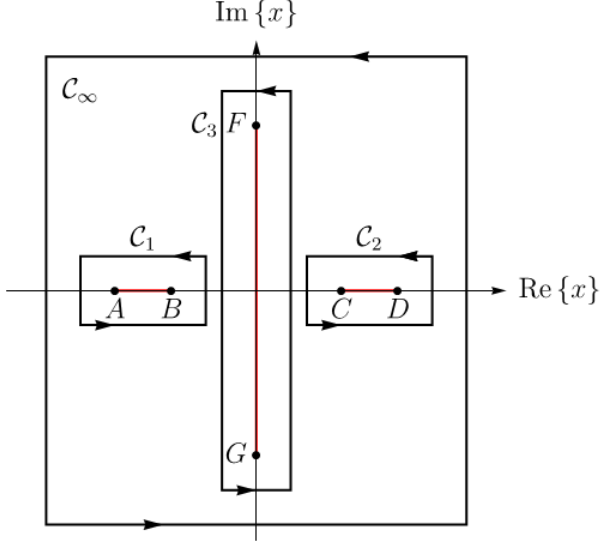


Figure 1: The integration contours for $\varrho_{\{\mu\}}(x, E)$.

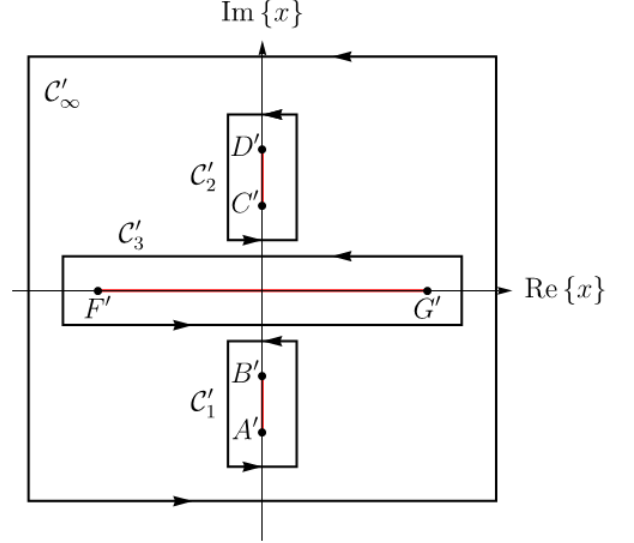


Figure 2: The integration contours for $\varrho_{\{-\mu\}}(x, E)$.

The sum of the integrals of $\varrho_{\{\mu\}}(x, E)$ over the contours \mathcal{C}_1 , \mathcal{C}_2 and \mathcal{C}_3 is equal to an integral over the large contour \mathcal{C}_∞ enclosing *all*⁵ the poles of $\varrho_{\{\mu\}}(x, E)$. The latter integral can be evaluated with aid of the residue of $\varrho_{\{\mu\}}(x,)$ at infinity:

$$2 \oint_{\mathcal{C}_1} \varrho_{\{\mu\}}(x, E) dx + \oint_{\mathcal{C}_3} \varrho_{\{\mu\}}(x, E) dx = \oint_{\mathcal{C}_\infty} \varrho_{\{\mu\}}(x, E) dx = 2\pi i \operatorname{Res}\{\varrho_{\{\mu\}}(x, E), \infty\} \quad . \quad (39)$$

Here we assume the point $x = \infty$ to be an isolated singularity, which is indeed the case for the considered QES potential, as was demonstrated in [10].

The equality (39) establishes a relation between the quantisation condition for a system described by the potential $V_{\{\mu\}}(x)$, with the energy set negative, and the quantisation condition for a system described by $V_{\{-\mu\}}(x)$, with the energy set positive. In other words, starting from (36), we can *derive* the quantisation condition in the form (34) for $V_{\{-\mu\}}(x)$.

To calculate the residue at infinity, we introduce the variable y :

$$y \equiv \frac{1}{x} \quad , \quad (40a)$$

$$\tilde{\varrho}_{\{\mu\}}(y, E) \equiv \varrho_{\{\mu\}}(1/y, E) \quad , \quad (40b)$$

in terms whereof the Ricatti equation (32) assumes the shape:

$$\tilde{\varrho}_{\{\mu\}}^2(y, E) + i y^2 \tilde{\varrho}'_{\{\mu\}}(y, E) = 2(E - V_{\{\mu\}}(1/y)) \quad . \quad (41)$$

⁵ Here we employ the fact that the function $\varrho_{\{\mu\}}(x, E)$ has no poles other than those inside the contours \mathcal{C}_1 , \mathcal{C}_2 or \mathcal{C}_3 . Indeed, as was demonstrated in [11], the poles of the QMF emerge only on the branch lines of the classical momentum, which in our case are the segments of the real and imaginary axes, enclosed by \mathcal{C}_1 , \mathcal{C}_2 and \mathcal{C}_3 .

The Laurent expansion for $\tilde{\varrho}_{\{\mu\}}(y, E)$ reads as

$$\tilde{\varrho}_{\{\mu\}}(y, E) = \sum_{k=-3}^{\infty} a_k y^k \quad . \quad (42)$$

The lowest power of y is determined by the highest power of x in $V(x)$ in (32). Substituting the above expansion into the integral (39) gives:

$$\oint_{C_{\infty}} \varrho_{\{\mu\}}(x, E) dx = \oint_{C_0''} \tilde{\varrho}_{\{\mu\}}(y, E) \frac{1}{y^2} dy = 2\pi i a_1 \quad , \quad (43)$$

where the contour C_0'' encloses the origin in the complex y -plane. To find a_0 , we insert the Laurent series (42) in the Ricatti equation (41) and match the coefficients of the five lowest powers of y :

$$\begin{aligned} k = -6 : & \quad \frac{\nu^2}{4} + a_{-3}^2 = 0 \\ k = -5 : & \quad 2a_{-3} a_{-2} = 0 \\ k = -4 : & \quad \frac{\nu \mu}{2} + a_{-2}^2 + 2a_{-3} a_{-1} = 0 \\ k = -3 : & \quad 2(a_{-3} a_0 + a_{-2} a_{-1}) = 0 \\ k = -2 : & \quad \frac{\mu^2}{4} - \frac{1}{2}(8j+3)\nu + a_{-1}^2 + 2a_{-2} a_0 + a_{-3}(2a_1 - 3i) = 0 \quad . \end{aligned} \quad (44)$$

The two sets of solutions are:

$$\left\{ \begin{array}{l} a_{-3} = -\frac{i\nu}{2} \\ a_{-2} = 0 \\ a_{-1} = -\frac{i\mu}{2} \\ a_0 = 0 \\ a_1 = i(4j+3) \end{array} \right. , \quad \left\{ \begin{array}{l} a_{-3} = \frac{i\nu}{2} \\ a_{-2} = 0 \\ a_{-1} = \frac{i\mu}{2} \\ a_0 = 0 \\ a_1 = -4ij \end{array} \right. \quad . \quad (45)$$

Following [10], we employ the condition of square integrability of the wave function

$$\psi(x) = \exp \left[i \int^x \varrho_{\{\mu\}}(\tilde{x}, E) d\tilde{x} \right] \quad . \quad (46)$$

For large x (and small y) one gets:

$$\psi(x) \approx \exp \left[i \frac{a_{-3} x^4}{4} \right] \quad , \quad (47)$$

and one has to choose the second set of solution with $a_{-3} = i\nu/2$ and $a_1 = -4ij$. This yields:

$$2 \oint_{c_1} \varrho_{\{\mu\}}(x, E) dx + \oint_{c'_3} \varrho_{\{-\mu\}}(x, -E) dx = \oint_{c_\infty} \varrho_{\{\mu\}}(x, E) dx = 2\pi i(-4ij) = 8\pi j \quad (48)$$

or, equivalently:

$$\oint_{c_\infty} \varrho_{\{\mu\}}(x, E) dx = 2\pi N \quad (\text{for } V_{\text{even}}) \quad , \quad (49)$$

where

$$N = 2J - 2 = 4j \quad (50)$$

is the number of the highest energy level in the algebraic sector. Moving the first integral, with an opposite sign, from the LHS to the RHS, and then using the equality (36), one arrives at

$$\oint_{c'_3} \varrho_{\{-\mu\}}(x, -E) dx = \oint_{c_\infty} \varrho_{\{\mu\}}(x, E) dx - 2 \oint_{c_1} \varrho_{\{\mu\}}(x, E) dx = 2\pi(N - 2m) \quad (\text{for } V_{\text{even}}) \quad . \quad (51)$$

From looking at the formulae (36) and (51), one may misconclude that the m -th energy level of the potential $V_{\{\mu\}}(x)$ is symmetric to the $(N - 2m)$ -th energy level of $V_{\{-\mu\}}(x)$. This, however, would be a mistake. There is a fundamental difference between the energies above the relative maximum of the potential, which we for now assume to be at $x = 0$, and those below. In the former case, the equation (36) has a single solution for the energy, while in the latter — two solutions:

$$\oint_{c_1} \varrho_{\{\mu\}}(x, E) dx = 2\pi m \quad \rightarrow \quad \begin{cases} E_{\{\mu\}, m} & \text{if } E_{\{\mu\}, m} > V_{\{\mu\}}(0) \\ E_{\{\mu\}, m(-)}, E_{\{\mu\}, m(+)} & \text{if } E_{\{\mu\}, m(+)} < V_{\{\mu\}}(0) \end{cases} \quad , \quad (52)$$

We intend to comply with a standard convention wherein (a) the notation $E_{\{\mu\}, n}$ stands for the n -th energy level from the bottom, and (b) the bottom level corresponds to $n = 0$. To that end, the energy levels below $V_{\{\mu\}}(0)$ should be enumerated as: ⁶

$$\begin{cases} E_{\{\mu\}, 2m} = E_{\{\mu\}m(-)} \\ E_{\{\mu\}, 2m+1} = E_{\{\mu\}m(+)} \end{cases} \quad \text{if } E_{\{\mu\}, m(-)} < V_{\{\mu\}}(0) \quad . \quad (53)$$

Now we see that $2m$ in the equation (51) is the number of the even energy level, $E_{\{\mu\}, 2m}$. In other words, for an even n , the n -th energy level is symmetric to the $(N - n)$ -th energy level:

$$E_{\{\mu\}, n} = -E_{\{-\mu\}, N-n} \quad , \quad n = 0, 2, 4, \dots, N \quad (\text{for } V_{\text{even}}) \quad . \quad (54)$$

It is worth noting that the energies $E_{\{\mu\}, m(-)}$ and $E_{\{\mu\}, m(+)}$ share a perturbative part and differ only due to the non-perturbative splitting called into being by the tunneling effects. These

⁶ Strictly speaking, (52) does not cover all the possibilities. A situation may emerge, wherein the highest level below $V_{\{\mu\}}(0)$ is $E_{\{\mu\}, m^*(-)}$, and it lacks a counterpart $E_{\{\mu\}, m^*(+)}$. Nonetheless, in this case the proper numbering is $E_{\{\mu\}, 2m^*} = E_{\{\mu\}, m^*(-)}$, as is (53).

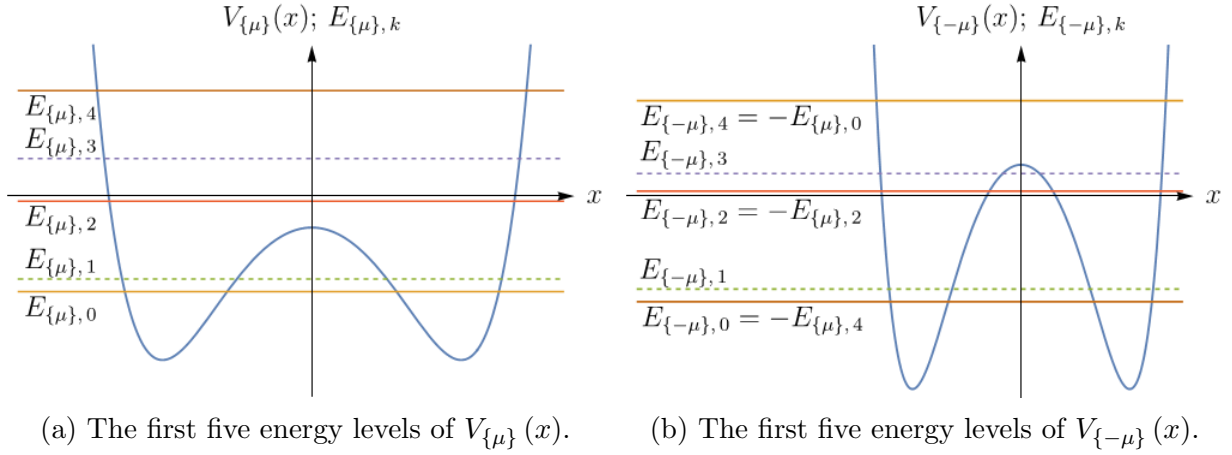


Figure 3: Typical spectra of $V_{\{\mu\}}(x)$, on the left pane, and of $V_{\{-\mu\}}(x)$, on the right pane. Both plots correspond to $j = 1$ (i.e., to $N = 4$). In both plots, even levels are depicted with solid lines, while odd levels are dashed.

effects get smaller near the bottom of the wells, and become strong closer to the maximum. At the perturbative level (in neglect of the splitting), one can say that the level $E_{\{-\mu\},N-n}$ is symmetric to two levels: $E_{\{\mu\},n}$ and $E_{\{\mu\},n+1}$.

For the odd potential (19b), integrating $\tilde{\varrho}_{\{\mu\}}(x, E)$ over the contour \mathcal{C}_∞ furnishes:

$$\oint_{\mathcal{C}_\infty} \tilde{\varrho}_{\{\mu\}}(x, E) dx = 2\pi(\tilde{N} + 1) \quad (\text{for } V_{\text{odd}}) \quad , \quad (55)$$

where the number of the highest energy level in the algebraic sector is now given by:

$$\tilde{N} = 2J - 1 = 4j + 1 \quad . \quad (56)$$

Then, starting again with (36), we arrive at:

$$\oint_{\mathcal{C}'_3} \tilde{\varrho}_{\{-\mu\}}(x, -E) dx = 2\pi(\tilde{N} - 2m) = 2\pi(\tilde{N} + 1 - (2m + 1)) \quad (\text{for } V_{\text{odd}}) \quad . \quad (57)$$

Be mindful that in the case of the odd potential, one chooses $\tilde{E}_{\{\mu\},m(+)} = \tilde{E}_{\{\mu\},2m+1}$ when solving (52). Therefrom, the energy spectrum reflection reads:

$$\tilde{E}_{\{\mu\},\tilde{n}} = -\tilde{E}_{\{-\mu\},\tilde{N}+1-\tilde{n}} \quad , \quad \tilde{n} = 1, 3, 5, \dots, \tilde{N} \quad (\text{for } V_{\text{odd}}) \quad . \quad (58)$$

As was already mentioned, the potentials $V_{\{\mu\}}(x)$ and $\tilde{V}_{\{\mu\}}(x)$ do not necessarily have a double-well form. Depending on the values of the parameters, they may have one, two or three minima. However, it turns out that for the energies in the algebraic sector the integration contours always look as in Figures 1 and 2.

The more surprising is that our result obtained by heavy-duty tools of Quantum Mechanics could have been proven in one line by using the Theorem from Section 1, as we have explained in the end of Section 2.1.

This example from Quantum Mechanics serves as a strong motivation to study the analytic properties of the potentials and the generalised WKB quantisation condition. For example, it turns out that the symmetry of the quantum energy levels has classical origins [12].

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